

Table S1. Calculated contributions to free energy of activation for *p*-CMP and *p*-MMP complexed with MAO B.

Substrate	Complex State	^a BBS	^b Solvation Effects		^c Thermal Correction and ZPE	^d Free Gibbs Energy		^e $\Delta G_{\epsilon=4}^{\ddagger}$	^e $\Delta G_{\epsilon=80}^{\ddagger}$
			$\epsilon = 4$	$\epsilon = 80$		$\epsilon = 4$	$\epsilon = 80$		
<i>p</i> -CMP	RC	- 5959.0633566	0.2196339	0.2918863	1.767073	- 5957.0766497	-5957.0043973	35.0	34.6
	TS	- 5959.0062118	0.2175651	0.2891722	1.767758	- 5957.0208887	-5956.9492816		
<i>p</i> -MMP	RC	- 5613.9583915	0.2295289	0.3019354	1.819695	- 5611.9091676	-5611.8367611	19.5	20.2
	TS	- 5613.9128681	0.2216267	0.2951898	1.81311	- 5611.8781314	-5611.8045683		

^aSingle point energy in hartrees at M06-2X/6-311+(2d,2p) level of theory (Big Basis Set).

^bSolvent contribution to the free Gibbs energy in hartrees calculated using $\epsilon=4$ and $\epsilon=80$.

^cThermal correction to the free Gibbs energy and Zero Point Correction in hartrees.

^dSum of BBS+Solvation+Thermal corrections terms in hartrees.

^eDifference between TS and RC free Gibbs energies in kcal/mol.

*Correspond to $G_{\text{Adduct}} - G_{\text{RC}}$ in kcal/mol.